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John H. Booske

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14. ABSTRACT
The results of this investigation have yielded two major new research capabilities and several important advances in physical understanding of materials and devices at high (THz-regime) frequencies. A quasi-optical cavity THz measurement system was developed with a record-high Q and resolution capable of measuring differences in surface conductivity less than 10% at frequencies between 300 – 1000 GHz. A multiphysics computational model (EMC, FDTD, MD) was developed for electron transport in solid conducting media under electromagnetic radiation driving forces. New discoveries were made about the losses of high frequency THz radiation in conducting media, including the effects of moderate conductivity (semi-conductors) and surface roughness. Experiments were also completed that characterized the effect of water vapor on atmospheric attenuation of THz radiation. Those data were in excellent agreement with the Millimeter-Wave Propagation Model, even though that model was originally developed for the lower millimeter-wave frequencies.

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Key Accomplishments

- Quasi-optical cavity THz measurement system was developed with a record-high Q and resolution capable of measuring differences in surface conductivity less than 10% at frequencies between 300 – 1000 GHz (currently operational at 400 and 650 GHz) [8,14, 28, 30, 32].
- Multiphysics model (EMC, FDTD, MD) was developed for electron transport under electromagnetic radiation driving forces, validated in comparisons with experimental data [1-3,7, 9-12, 14-16, 18, 24, 26, 28-30]. A determination was made that the Drude model is not sufficiently accurate for describing the high frequency bulk conductivity of semi-conducting materials, at least for mobile charge carrier densities up to 10^{14} cm^{-3}. Probable reason is the inadequacy of the assumption of quasi-static conditions ($\omega\tau << 1$, τ being the relaxation time) at such high frequencies. [2,3, 7, 9-12, 14-16, 18, 24, 26, 28-30, 34]
- Experiments were completed that characterized the effective conductivity of doped semiconductors, as a function of dopant density [14, 18, 24, 27, 28, 30, 32].
- Experiments were conducted that characterized the effect of surface topography (roughness) on THz radiation losses in metallic conductors [20, 22, 25, 27, 30, 32]. The results revealed that surface roughness losses are generally higher than predicted by available models, and that the losses have different dependencies on the average feature size of the roughness depending on whether the roughness is regular or random.
- Experiments were conducted that characterized the effect of water vapor on atmospheric attenuation of THz radiation [17, 19, 21, 23, 33]. The data reveal that the widely-used Millimeter-Wave Propagation Model (MPM), extrapolated to the THz regime, provides accurate predictions of losses due to water vapor.
- Theoretical model was developed and validating experiments were conducted that explain the reason for step frequency tuning observed with THz regenerative TWT oscillators. [4-6,13].
- Comprehensive assessment was made of high power sources in the THz regime [6, 27].

- Booske was elected Fellow of the American Physical Society "For pioneering contributions to the development of coherent radiation sources in the submillimeter wave and terahertz regime, in particular to the physics of sheet electron beams, advanced cathode, and interaction of high power microwave with materials."

Archival Publications (published)

Peer reviewed full papers

[1] K.J. Willis, S.C. Hagness, and I. Knezevic, "A global EMC/FDTD simulation tool for high-frequency carrier transport in semiconductors," 13th International Workshop on Computational Electronics, (full length conference paper) Beijing, China, May 2009, pp. 265-268. Available online through IEEE Xplore. http://dx.doi.org/10.1109/IWCE.2009.5091080

[2] K. Willis, J. Ayubi-Moak, S. C. Hagness, and I. Knezevic, "Global modeling of carrier-field dynamics in semiconductors using EMC-FDTD," *Journal of Computational Electronics*, vol. 8, pp. 153-171, August 2009.

[3] K. J. Willis, S. C. Hagness, and I. Knezevic, "Terahertz conductivity of doped silicon calculated using the ensemble Monte Carlo/finite-difference time-domain (EMC/FDTD) simulation technique," *Applied Physics Letters*, vol. 96, no. 6, 062106, February 8, 2010.

[4] P. Gao, J.H. Booske, Z.H. Yang, "Frequency step-tuning characteristics of traveling-wave tube regenerative oscillators," *IEEE Trans Elec Dev*, vol 57, 1152-1159 (2010).

[5] P. Gao, J. H. Booske, Z.-H. Yang, B. Li, J. He, Y.-B. Gong, Z. Tian, "Physics and Simulation of Terahertz Folded Waveguide Traveling Wave Tube Regenerative Feedback Oscillators," *Acta Physica Sinica*, Vol.59, No.12, pp. 8484-8489 (2010, in Chinese).

[6] J. H. Booske, R. J. Dobbs, C. D. Joye, C. L. Kory, G. R. Neil, G.-S. Park, J. Park, and R. J. Temkin, "Vacuum Electronic High Power Terahertz Sources," **invited review paper**, Inaugural Issue, *IEEE Transactions on Terahertz Science and Technology*, Vol. 1, No. 1, pp. 52-75 (2011).

[7] K.J. Willis, S.C. Hagness, and I. Knezevic, "Multiphysics simulation of high-frequency carrier dynamics in conductive materials," J. Appl. Phys. **110**, 063714 (2011).

Conference Abstracts and Talks

[8] B.B. Yang, K.J. Willis, I. Knezevic, S.C. Hagness, F. Cerrina, D.W. van der Weide, J.H. Booske, "Fundamental electronic properties of materials for terahertz vacuum electron devices," IEEE 35th International Conference on Plasma Science, Karlsruhe, Germany, 2008.

[9] K.J. Willis, S.C. Hagness, and I. Knezevic, "A global EMC/FDTD simulation tool for modeling THz wave interaction with conductive media," American Physical Society March Meeting, Pittsburgh, PA, March 2009.

[10] K.J. Willis, S.C. Hagness, and I. Knezevic, "A global EMC/FDTD simulation tool for high-frequency carrier transport in semiconductors," 13th International Workshop on Computational Electronics (IWCE), Beijing, China, May 27-29, 2009.

[11] K. J. Willis, S. C. Hagness, and I. Knezevic, "A Combined EMC-FDTD Solver for Terahertz Characterization of Doped Silicon," IEEE International Symposium on Antennas and Propagation and USNC/URSI National Radio Science Meeting, Charleston, SC, June 1-5, 2009.

[12] K. J. Willis, I. Knezevic, and S. C. Hagness, "A multiphysics numerical technique for THz-frequency carrier transport in semiconductors and metals," American Physical Society March Meeting, Portland, OR, March 2010.

[13] Peng Gao, John H. Booske, and Zhonghai Yang, "Transient and Steady State Operation of Traveling Wave Tube Regenerative Oscillators," 11th IEEE International Vacuum Electronics Conference, Monterey, CA (May 18-20, 2010).

[14] B.B. Yang, S.L. Katz, K.J. Willis, I. Knezevic, S.C. Hagness, J.H. Booske, "Characterizing electronic properties of low and high conductivity materials in the THz regime," *2010 35th International Conference on Infrared, Millimeter, and Terahertz Waves* (IRMMW-THz, Rome, Sept 5-10, 2010), Conference Guide, Mo-P.36

[15] K.J. Willis, S.C. Hagness, and I. Knezevic, "EMC/FDTD/MD for Multiphysics Characterization of Semiconductors at THz Frequencies," 14th International Workshop on Computational Electronics (IWCE 2010), Pisa, Italy, October 27-29, 2010.

[16] K.J. Willis, I. Knezevic, and S.C. Hagness, "Multiphysics Computational Solver for THz-Frequency Characterization of High-Conductivity Materials," 2010 IEEE AP-S International Symposium on Antennas and Propagation and 2010 USNC/CNC/URSI Meeting in Toronto, ON, Canada, July 11-17, 2010.

[17] M. J. Weber, B. B. Yang, S. L. Katz, J. H. Booske, "Characterization of Electromagnetic Losses in the Terahertz Regime Due to Atmospheric Water Content," *USNC-URSI National Radio Science Meeting* (Boulder, CO, January 5-8, 2011) paper F2-9

[18] B. B. Yang, S. L. Katz, K. J. Willis, I. Knezevic, S. C. Hagness, and J.H. Booske, "Experimental Characterization of Doped Silicon Conductivity in the Terahertz Regime with a High-Q Quasioptical Resonator," *USNC-URSI National Radio Science Meeting* (Boulder, CO, January 5-8, 2011) paper A4-1

[19] M. J. Weber, B. B. Yang, S. L. Katz, J. H. Booske, "Investigation of the Attenuating Effects of Atmospheric Water Content at 400 GHz," *IEEE International Vacuum Electronics Conference*, (Bangalore, India, Feb 21-24, 2011).

[20] B.B. Yang and J.H. Booske, "Measurement of Surface Roughness Effects on Conductivity in the Terahertz Regime, with a High-Q Quasioptical Resonator," IEEE Int'l Conf. Plasma Sci., Chicago, IL, June 26-30, (2011), paper IO2B-4.

[21] M.J. Weber, B.B. Yang, S.L. Katz, and J.H. Booske, "Examination of Electromagnetic Attenuation Induced by Atmospheric Water Content on Terahertz Radiation," IEEE Int'l Conf. Plasma Sci., Chicago, IL, June 26-30, (2011), paper IO2B-7.

[22] Matthew Kirley, Benjamin Yang, John Booske, "Study of the Effect of Nanofabricated Surface Roughness on Conductivity in the Terahertz Regime with a High-Q Resonator," 36th Int'l Conf. Infrared, Millimeter and Terahertz Waves, paper M2C.3 (Houston, TX, Oct 2-7, 2011).

[23] Marcus Weber; Benjamin Yang; Mark Kulie; Ralf Bennartz; John Booske, "Analysis of Atmospheric Attenuation due to Water Content at 400 and 650 GHz," 36th Int'l Conf. Infrared, Millimeter and Terahertz Waves, paper M3B.3 (Houston, TX, Oct 2-7, 2011).

[24] Matthew Kirley; Benjamin Yang; Keely Willis; Marcus Weber; Nishant Sule; Susan Hagness; Irena Knezevic; John Booske, "Measurements of Near Terahertz Conductivity of Doped Silicon using a High Quality Factor Resonant Cavity," 36th Int'l Conf. Infrared, Millimeter and Terahertz Waves, paper W5.20 (Houston, TX, Oct 2-7, 2011).

[25] B.B. Yang, J.H. Booske, M. Kirley, "Effect of Surface Roughness on Metallic Conductivity in the Terahertz Regime," 53rd Annual Mtg American Phys. Soc. Div. Plasma Physics, paper T07.3 (Salt Lake City, Utah, (Nov. 14-18, 2011).

[26] K. Willis, I. Knezevic, and S.C. Hagness, "A multiphysics computational technique for THz-frequency characterization of semiconductors and metals," 2011 XXXth URSI General Assembly and Scientific Symposium, Istanbul, Turkey, (2011).

[27] John H. Booske, "Vacuum Electronic Sources of High Power Terahertz-Regime Radiation," Invited Plenary Talk, IEEE International Conference on Vacuum Electronics, Bangalore, IN, February 21-25, 2011.

Ph.D. and M.S. Reports and Theses

[28] S.L. Katz, "Near Terahertz Silicon Conductivity Measurements via High Q Resonant Cavity," M.S. report (unpublished), University of Wisconsin-Madison, 2010.

[29] K.J. Willis, “A combined EMC-FDTD solver for simulation of terahertz-frequency wave interactions in conductive media,” Ph.D. thesis, University of Wisconsin-Madison, 2010.

[30] B.B. Yang, “The Effect of Surface Roughness on the Conductivity of Metals in the Terahertz Regime,” Ph.D. Thesis, University of Wisconsin-Madison, 2011.

In Preparation

Peer-reviewed Full Papers:

[31] R. Jacobs, J.H. Booske, D. Morgan, “Intrinsic Defects and Conduction Characteristics of Sc_2O_3 in Thermionic Cathode Systems: an *Ab Initio* Study, (in preparation, 2011).

[32] B. B. Yang, S. L. Katz, K. J. Willis, M.J. Weber, I. Knezevic, S. C. Hagness, and J. H. Booske, “Measurement of Electronic Properties of Conductors and Low-Loss Dielectrics with a High-Q Quasi-Optical Resonator, *IEEE Trans. THz Sci Technol.* (in preparation, 2011).

[33] M. J. Weber, B. B. Yang, M. Kulie, R. Bennartz, and J. H. Booske, “Atmospheric Attenuation of 400 GHz Radiation due to Water Content,” *IEEE Trans. THz Sci. Technol.* (submitted, 2011).

[34] K.J. Willis, S.C. Hagness, and I. Knezevic, “THz Conductivity of Silicon,” in preparation (2011).

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